GSFC · 2015

Computational Investigation of Ignition Delay for Various Fuels in a Heated Cavity-Stabilized Combustor

Cameron Butler and Stuart Laurence
University of Maryland – College Park

Presentation Overview

- Research goals
- Computational tools and methodology
- Simulation Results
- Research Findings/Conclusions
- Future Plans

Research Motivation

CHALLENGES

- Supersonic combustion in scramjet combustors requires mixing and ignition on very short time-scales; cavity flameholders used for flame stabilization
- Combustor walls in short-duration test facilities remain much colder than temperatures experienced during flight
- For lower Mach numbers, focus is shifting from hydrogen to hydrocarbon fuels (e.g., X-51)
- Hydrogen ignition is typically easily achieved, but hydrocarbon ignition delay times can be on the order of the flow residence time; cold walls may increase this further

Research Motivation

CHALLENGES

•Supersonic combustion in scramjet combustors requires mixing and ignition on very short time-scales; cavity flameholders used for flame stabilization

•Combustor walls in short-duration test facilities remain much colder than temperatures experienced during flight

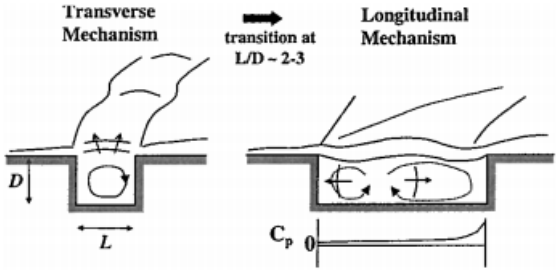
•For lower Mach numbers, focus is shifting from hydrogen to hydrocarbon fuels (e.g., X-51)

•Hydrogen ignition is typically easily achieved, but hydrocarbon ignition delay times can be on the order of the flow residence time; cold walls may increase this further

PURPOSE

•Characterize ignition behavior in a supersonic cavity-stabilized combustor

- Determine effect of wall pre-heating on ignition behavior
- Predict ignition behavior based on computationally inexpensive unreacting simulations
- Examine flow topology as a function of aspect ratio and wall temperature

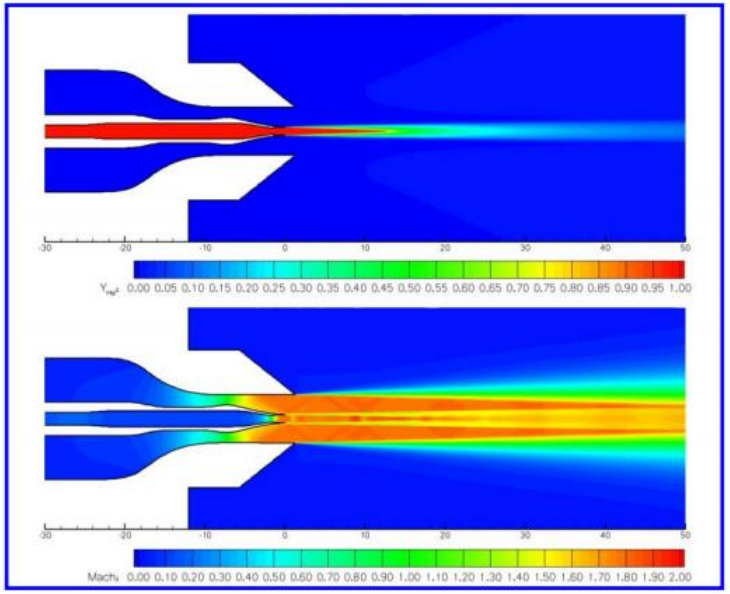


(Ben-Yakar and Hanson, 2001)

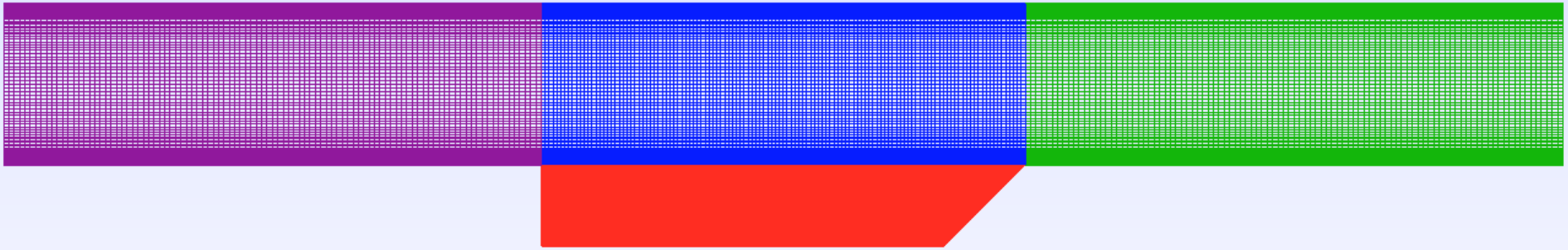
VULCAN-CFD

- Viscous Upwind Algorithm for Complex Flow Analysis
- Developed by the Hypersonic Air breathing Propulsion Branch of NASA Langley Research Center
- Steady-state and unsteady turbulent flow solver
- Capable of non-equilibrium, finite rate chemical kinetics
- Supports 2D, axisymmetric and 3D structured grids
- Variety of turbulence models including:
  - Wilcox k-ω (1998) – used for this study
  - Menter k-ω (SST)
  - Spalart-Allmaras

VULCAN simulation of coaxial supersonic free-jet simulation using Wilcox (1998) k-ω (Baurle and Edwards, 2009)



Computational Domain



Nodes		
	Unreacting	Reacting
L/D = 4.5	40,000	57,500
L/D = 5.5	45,652	56,964
L/D = 6.5	46,000	56,964
L/D = 8.5	60,000	93,208

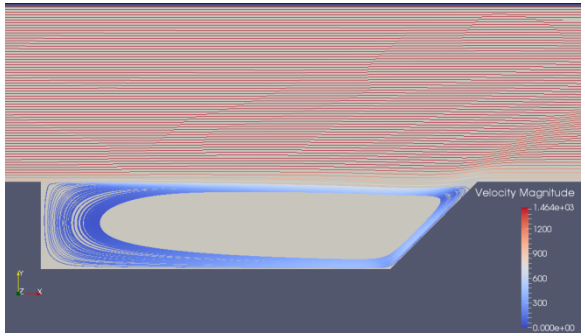
- Cavity geometry with L/D = 5.5 shown
- All grids generated using gmsh in 2D
- 100 mm inlet duct; 15 mm deep cavity
- Fully turbulent inflow
- No-slip walls; Top wall is symmetry plane

Testing Conditions

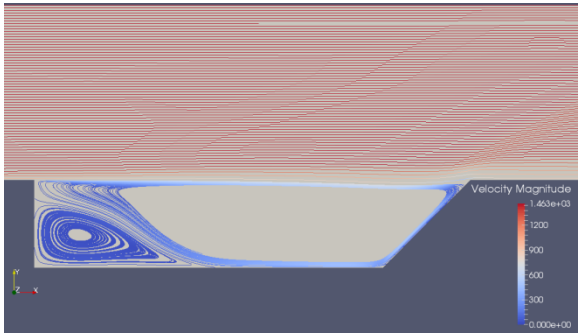
- Stagnation temperatures considered – 1600K, 1850K
- Inlet Mach 2.8; Static pressure 0.5 bar
- Turbulent Schmidt and Prandtl number – 0.9
- Six unique conditions for cavity walls:
  1. All walls held at 300K
  2. Bottom wall held at 700K or 900K, side walls at 300K
  3. All walls held at 700K, 900K or adiabatic (roughly 1450K)
- 900K max wall temperature and 1850K max stagnation temperature were chosen for experimental practicality
- Fuel equivalence ratio for reacting simulations – 0.2

Wall Conditions:

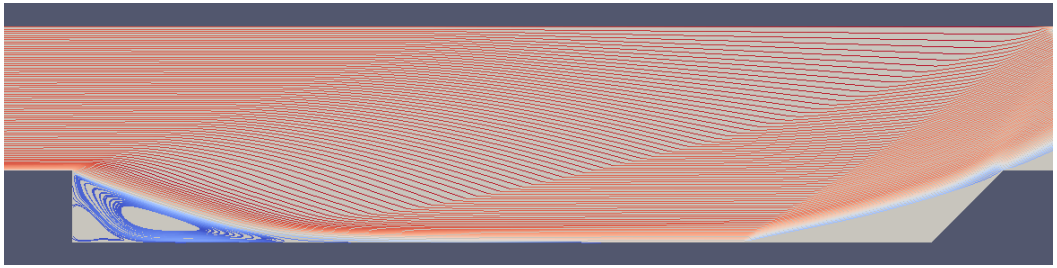
Varying Flow Topology



$L/D=4.5$, $T_0 = 1600K$
Cavity Temp = 300K



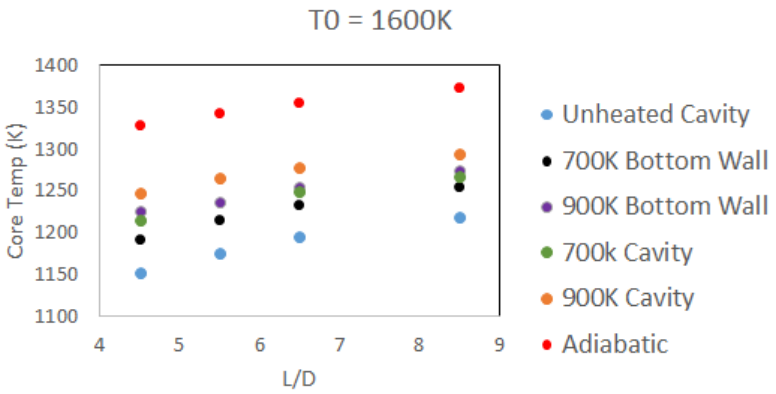
$L/D=4.5$, $T_0 = 1600K$
Adiabatic Cavity

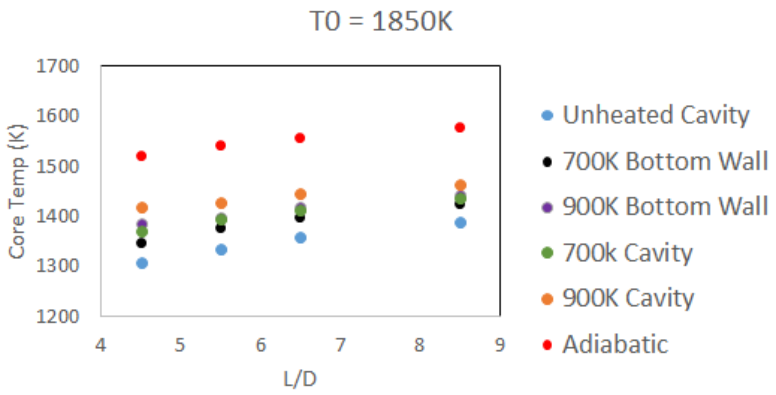


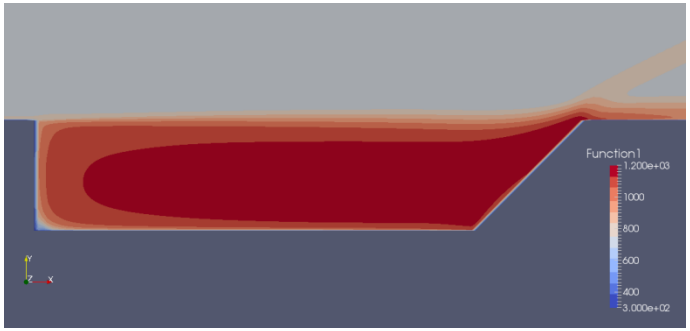
$L/D=12.5$, $T_0 = 1600K$, Cavity Temp = 300K

- According to Ben-Yakar and Hanson, topology influenced by inlet Mach, leading-edge boundary layer thickness, cavity aspect ratio and cavity width
- Wall temperature seems to have a strong impact as well
  - Hotter boundary layer becomes thicker and more prone to separation
- Could impact residence time and fuel distribution
- Transition from open to closed cavity at high aspect ratio

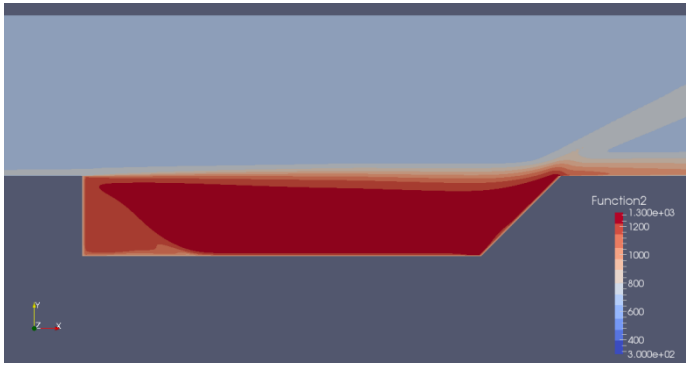
Steady-State Core Temperature







L/D=4.5, Cavity Temp = 300K, T_0 = 1600K



L/D=5.5, Cavity Temp = 900K, T_0 = 1600K

- Core temperature determined using two area-weighted averages
- Core flow temperature increases with cavity aspect ratio
- Pre-heating cavity to 900K more effective than doubling aspect ratio
- Ratio between core area and total cavity area decreases with increasing AR
- Temperature distribution is also topology-dependent

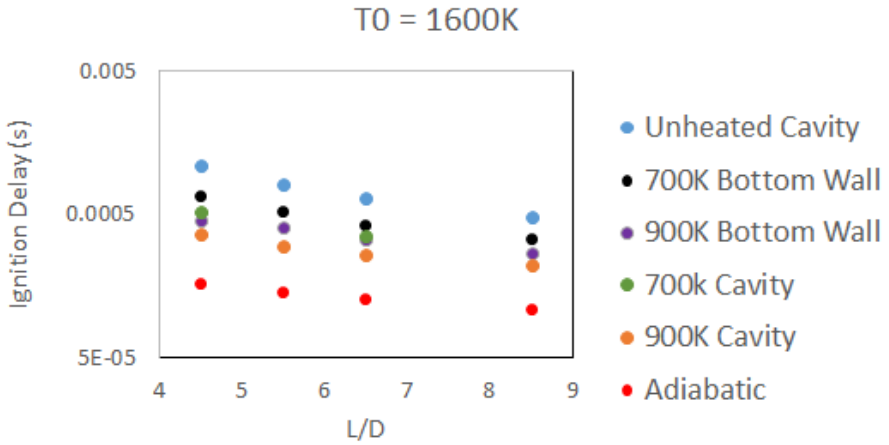
Ignition Delay

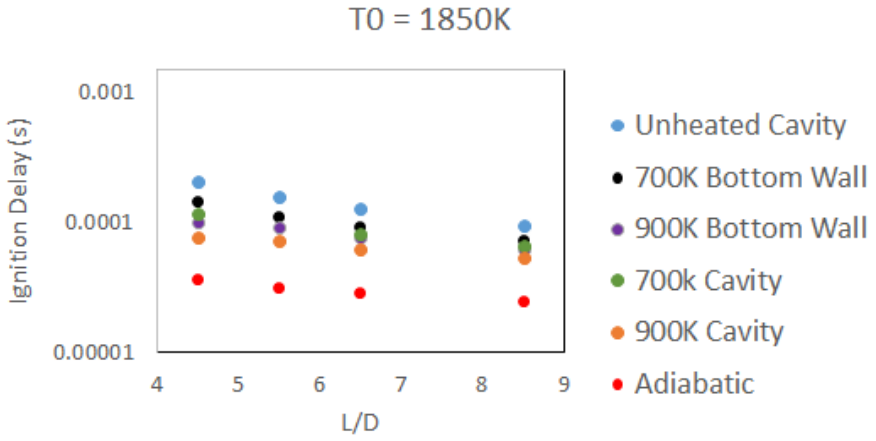
- Time for ignition to occur can be approximated by following equation developed by Colket and Spadaccini:

$$\tau = Aexp\left(\frac{E}{RT}\right)[O_2\ ]^{-1.2}[C_2H_4\ ]^0$$

where A is a constant, E is equivalent to global activation energy, R is the universal gas constant and terms in brackets are molar concentrations in mol/cc

- For ethylene, the ignition delay only indirectly depends on fuel concentration
- Core temperature for each operating condition can be combined with an assumed equivalence ratio to approximate ignition delay
- Note that correlation was developed using data with temperature range 1125-1410K

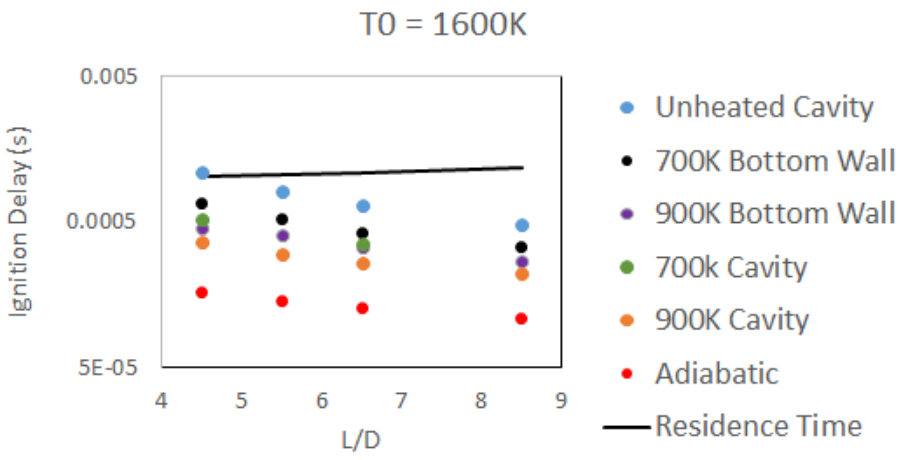


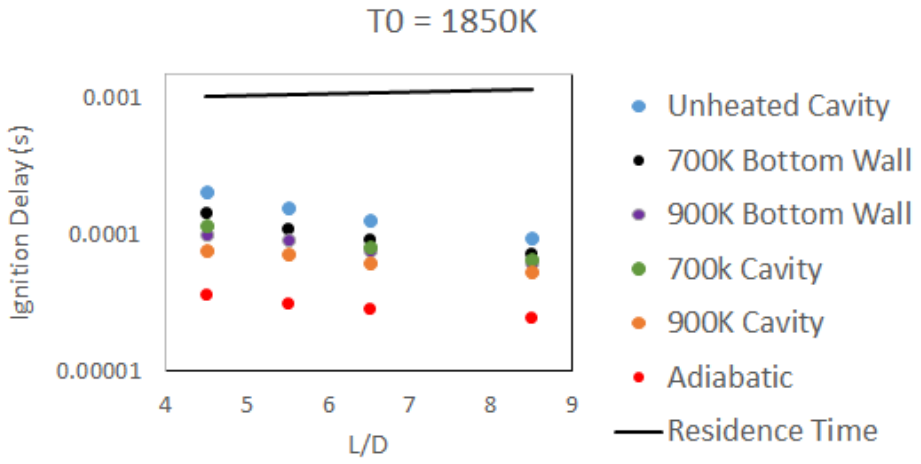


Flow Residence Time

- Air within cavity at steady state can be “tagged”
- Global time-stepping can then be used to calculate cavity air remaining within the cavity after a time
- Decay rate of cavity air assumed to follow exponential curve
- Cavity Residence time computed from following equation:

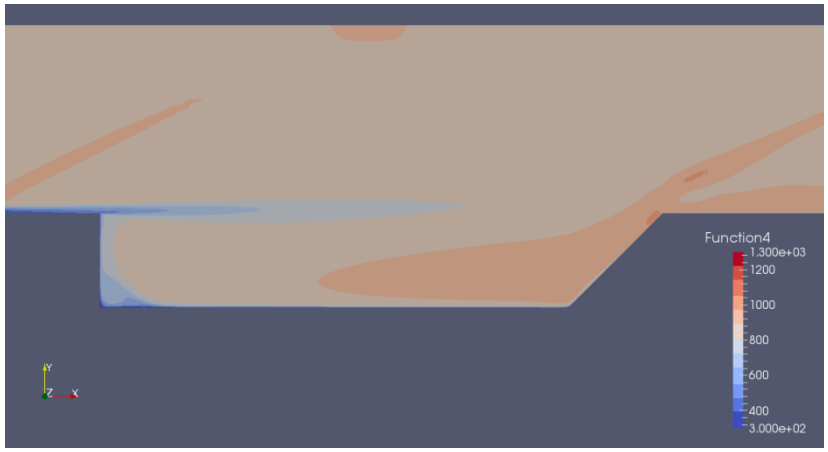
$$\tau = \frac{\Delta t}{\ln(\frac{M_1}{M_2})}$$ where M1 and M2 are the integrated mass fractions of remaining cavity air



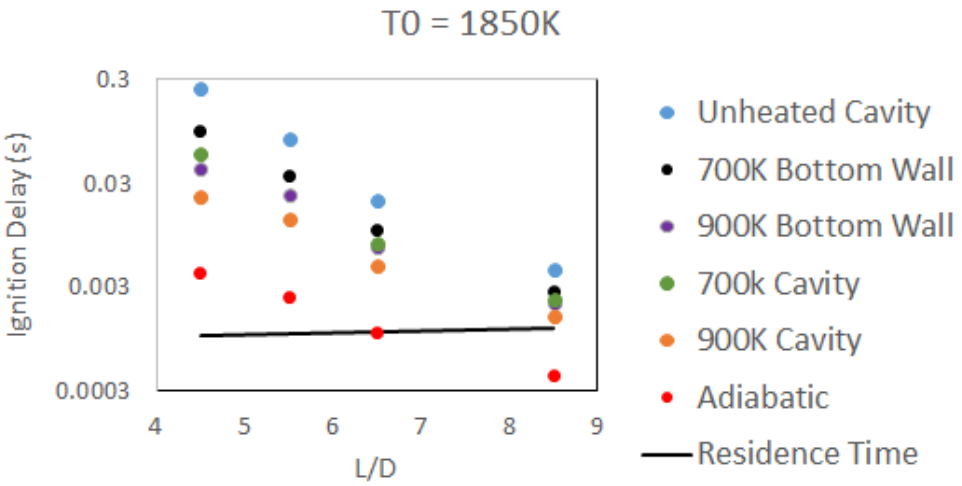


Effect of Fuel Temperature

- By running a non-reacting simulation with fuel injection, the impact of cold fuel on core temperature is determined
- Core temperature decreases by 350-470K, drastically increasing ignition delay
- Core temperature decreases less as aspect ratio increases
- After correction, a more conservative prediction of ignition is attained



L/D=5.5, Cavity Temp = 300K, T_0 = 1850K



Jachimowski Ethylene Reaction Mechanism

- 10 elementary reactions
- 10 chemical species
- Reaction rate determined by:

$$k_f = AT^B e^{-T_a/T}$$

where A, B and T_a are constants for each reaction and T is static temperature

$$C_2H_4 + O_2 \leftrightarrow 2H_2 + 2CO \qquad OH + H_2 \leftrightarrow H + H_2O$$

$$CO + O + M \leftrightarrow CO_2 + M \qquad H_2 + O \leftrightarrow H + OH$$

$$CO + OH \leftrightarrow CO_2 + H \qquad OH + OH \leftrightarrow H_2O + O$$

$$H_2 + O_2 \leftrightarrow 2OH \qquad H + OH + M \leftrightarrow H_2O + M$$

$$H + O_2 \leftrightarrow O + OH \qquad H + H + M \leftrightarrow H_2 + M$$

Ethylene Ignition (H_2O Mass Fraction), T_0 = 1600K

L/D=6.5, Cavity Temp = 300K

L/D=6.5, Cavity Temp = 900K

L/D=6.5, Adiabatic Cavity

Ethylene Ignition (H_2O Mass Fraction), T_0 = 1850K

L/D=4.5, Cavity Temp = 300K

L/D=4.5, Cavity Temp = 900K

L/D=4.5, Adiabatic Cavity

Ethylene Ignition (H_2O Mass Fraction), T_0 = 1850K

L/D=5.5, Cavity Temp = 300K

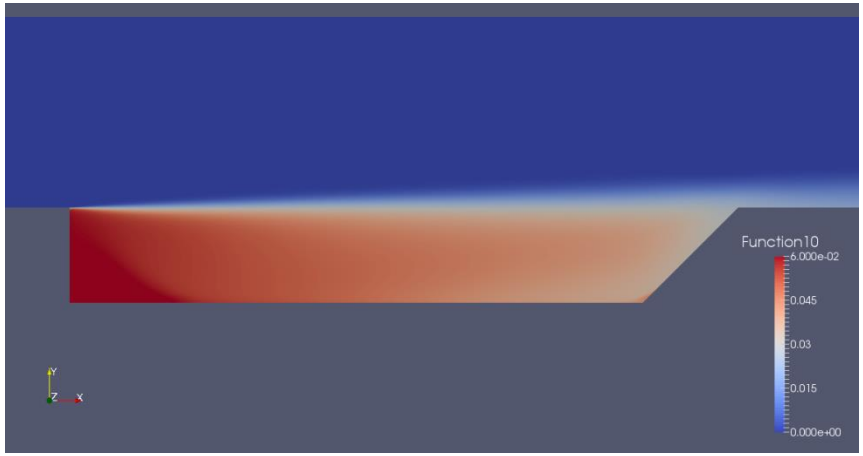
L/D=5.5, Cavity Temp = 900K

L/D=5.5, Adiabatic Cavity

Ethylene Ignition (H_2O Mass Fraction), T_0 = 1850K

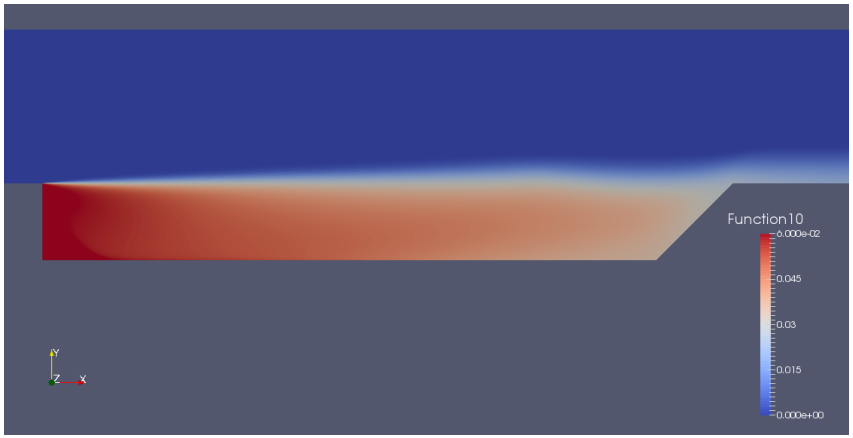
L/D=6.5, Cavity Temp = 300K

L/D=6.5, Cavity Temp = 900K

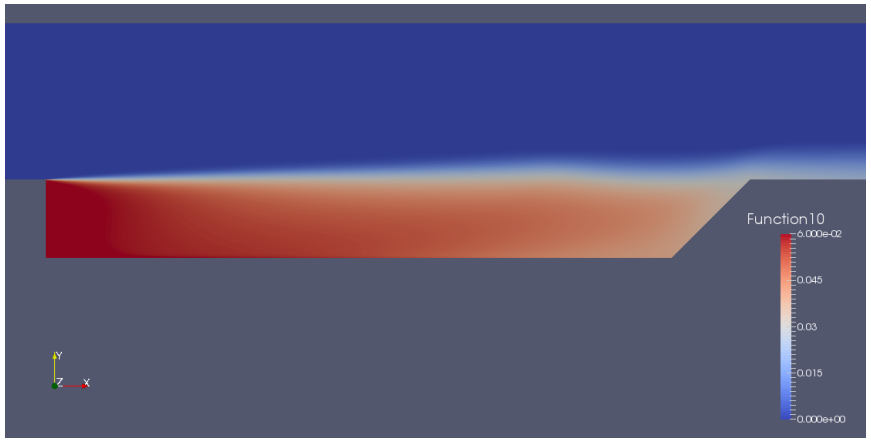


L/D=6.5, Adiabatic Cavity

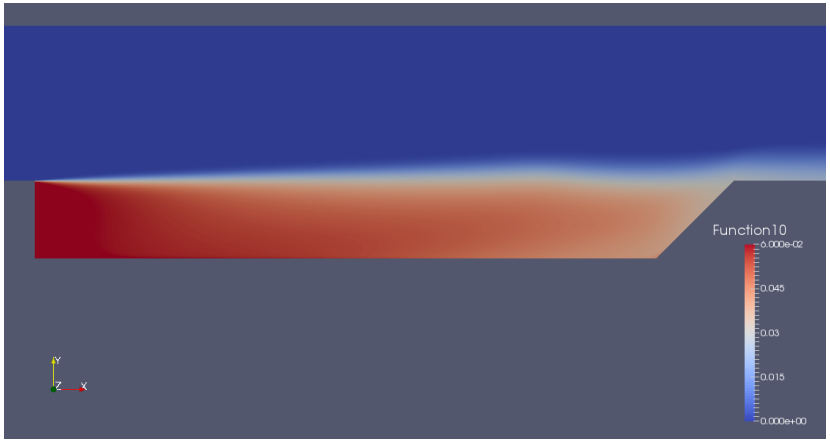
Ethylene Ignition (H_2O Mass Fraction), T_0 = 1850K



L/D=8.5, Cavity Temp = 300K



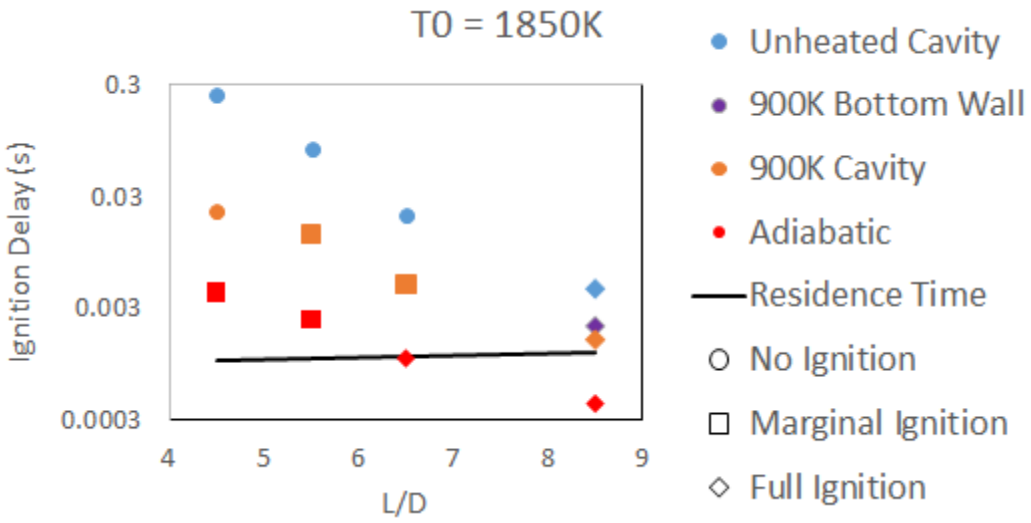
L/D=8.5, Bottom Wall = 900K



L/D=8.5, Cavity Temp = 900K

Ignition Summary

- Simulations results are shown differentiated based on ignition characteristics
- Circles indicate ignition was not achieved, squares indicate marginal ignition and diamonds indicate full ignition
- Ignition delay serves as a general guide for determining the ignition limits, but cannot be relied upon to perfectly predict ignition behavior
- Exponential temperature dependence makes prediction difficult



Conclusions

- Jachimowski reaction mechanism displays ignition behavior similar to that reported by Colket and Spadaccini based on computed residence time when fuel temperature is accounted for
- Pre-heating cavity walls tends to be a relatively weak factor for achieving ignition, but can be significant at the ignition limits
- Ignition behavior in a short-duration test facility without pre-heating can differ greatly from ignition behavior in-flight for specific conditions
- Increasing cavity aspect ratio assists in achieving ignition
- Corner recirculation zone acts as an anchoring point for ignition in otherwise ignition-free cases
- Non-uniform fuel distribution within cavity impacts ignition behavior

Future Work

- Investigate effects of lowering inlet Mach while keeping stagnation temperature constant, which will increase static temperature
- Study ignition behavior of additional fuels (methane, JP-10)
  - Ethylene has significantly lower activation energy than other hydrocarbon fuels
- Run reacting simulations using other ethylene reaction mechanisms
- Examine the impact of three-dimensional and axisymmetric flow features on ignition behavior
- Perform time-accurate simulations to determine importance of transients